Science and Engineering Supported by PETSc

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Summary

Partial differential equations (PDEs) are used to mathematically model phenomena in virtually all areas of science and engineering, from brain surgery to rocket science. We are developing the Portable, Extensible Toolkit for Scientific Computing (PETSc) to support high-performance simulations based on PDEs. The parallel computing infrastructure and scalable numerical solvers in PETSc enable scientists and engineers to focus on their primary scientific interests, thereby reducing implementation costs. PETSc helps hundreds of science and engineering groups to accomplish their work both faster and better.

Numerous ongoing application projects use various facets of PETSc. We highlight seven recent projects. All have resulted in scientific and engineering advances as chronicled in software and publications. References for these, as well as many others, may be found at our web site: www.mcs.anl.gov/petsc/petsc-as/publications

Fusion. Fusion uses the combination of hydrogen atoms to produce vast amounts of energy (for example, in our Sun) without the need for dangerous radioactive materials. Mathematical models for fusion are extremely complicated and difficult to solve but likely hold the key for learning to harness fusion energy for practical use.

Gyrokinetic simulation is one particular facet of computational fusion in which PETSc has been employed. This work involves the careful simulation of the dynamics of the electrons as they circle a toroidal chamber (the location where the fusion process is occurring). PETSc has also been used in other aspects of fusion simulation, including plasma models using both spectral and finite element methods.

Environmental Science. The Department of Energy (DOE) has an enormous interest in better understanding *subsurface flow*, the flow of water and other substances through the ground, for example, toward water wells. The reason is DOE is responsible for cleaning its legacy of contaminated sites across the country, a multibillion dollar endeavor. An example of this work is the LANL report *Modeling Thermal-Hydrological-Chemical (THC) Coupled Processes with Applications to Underground Nuclear Tests at the Nevada Test Site,* which is based on computations done using the PETSc software library.

Biological/Medical Applications. Advances in biological understanding and medical advances are proliferating as the direct result of mathematical models and numerical simulations. During the past year the PETSc software package and our expertise have been used for modeling and understanding *heart arrhythmias*. These

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disorders of the regular rhythmic beating of the heart cause the majority of sudden cardiac deaths.

Treating *fractures of the hip and spine* is a major medical cost. Understanding bone mechanical properties and how they may lead to fractures is thus an important medical research activity. A team of physicians and computational scientists have used PETSc and the software package Prometheus for simulations of hips and spines. This computation was a winner of a Gordon Bell Special Prize at SC2004 and ran scalably on over 4,000 processors.

MRIs and CT scans have had an enormous impact on the quality of medical care that is delivered today, but they still have limitations on the resolution of the images they can produce. Researchers are using PETSc to determine how to produce higher-quality imaging algorithms.

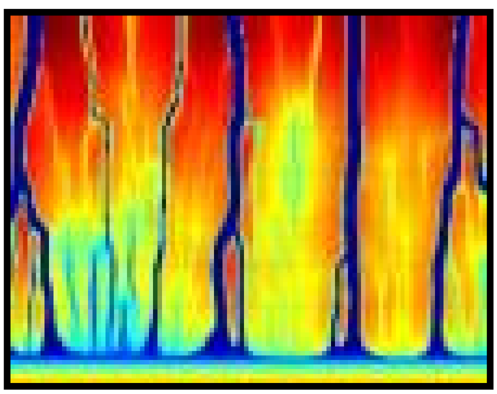

Fig. 1. Melt channels in magmatic reactive flow in porous ascent up a solubility gradient

Geosciences. The modeling of log-term *geodynamics* is crucial, not only for energy exploration and exploitation, but for a more fundamental understanding of processes involved. Researchers at Columbia University have used PETSc to explore the coupling between regional mantle subduction and the reactive flow of hydrous magma in the lithosphere, see Fig. 1.

A key component to the reactive flow simulation is the introduction of a semi-Lagrangian advection solver. By eliminating numerical diffusion, we were able to resolve the advective dynamics, see Fig. 2. This functionality has been packaged as a component and incorporated into PETSc, allowing any field to be advected precisely.

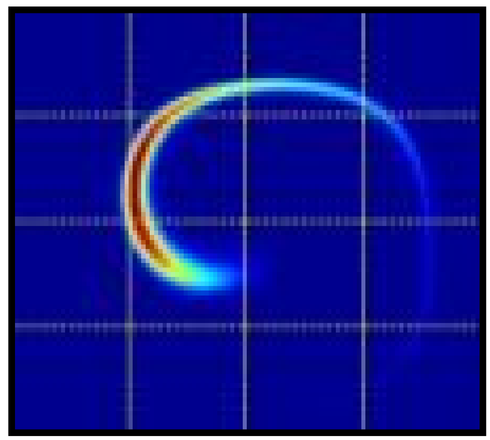

Fig. 2. Sharp features can easily be resolved using semi-Lagrangian advection solvers

Ship-Sea Interaction Modeling. The U. S. Navy has a strong interest in the simulation of ships and submarines moving through the ocean. The software package CFDShip-Iowa was recently enhanced to use PETSc for its algebraic solver needs. This package is a multiblock free surface flow solver that uses overset structured meshes, designed for ship applications. It has been used in the past year for "roll for surface combatant", for "beveled-trailing edge flows and wakes" and for "non-body-of-revolution" submarines as well as other applications.

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